Indian J. Phys. **70B** (6), 459–463 (1996)

IJP B
- an international journal

Multi parameter Rayleigh-Schrödinger perturbation theory

Nazakat Ullah*
Tata Institute of Fundamental Research, Homi Bhabha Road,
Colaba, Bombay-400 005, India

Received 10 May 1996, accepted 12 September 1996

Abstract : A new form of Rayleigh-Schrödinger (R-S) perturbation theory is given It has the usual advantage of R-S perturbation but gives more accurate values of perturbed eigenvalues than Brillouin-Wigner (B-W) perturbation theory. The modification is carried out in two steps The essential idea is to introduce a set of variational parameters in unperturbed Hamiltonian and use them to make the odd terms vanish Applied to anharmonic oscillator, the ground state energy upto third order is obtained with an accuracy of 0 45% while the first excited state calculated upto third order has an accuracy of 0 17%

Keywords : Perturbation theory, anharmonic oscillator

PACS No. : 03.65 Ge

1. Introduction

The perturbation theory has been extensively used in many areas of physics as the exact analytic solution of the Hamiltonian of these systems cannot be found. In the literature [1] the two most commonly used forms are : (1) Rayleigh-Schrödinger (R-S) perturbation theory and (2) Brillouin-Wigner (B-W) perturbation theory, both having some advantages and disadvantages from the practical point of view, *e.g.*, in R-S theory one uses unperturbed energies in all orders which is a great advantage but then the convergence is slower while in B-W, one uses exact value of the perturbed energy in all orders which is a disadvantage but its convergence is faster. The need for modifying perturbation theory was felt when the eigenvalues of the anharmonic oscillator with the anharmonic term λx^4 were needed as the terms of the perturbation series become larger and larger as the coupling parameter $\lambda \to \infty$. Even though there are techniques available to sum divergent series [2], it is more useful to modify the perturbation theory so that its first few order terms give a fairly accurate value of the calculated eigenvalues.

*e-mail nu @ tifrvax. tifr. res. in

The purpose of the present work is to reformulate R–S theory to achieve such a goal. In the process, we shall show that R–S theory upto second order gives the same result as B–W theory in which exact energy is replaced by zero-order B–W theory. We describe the formulation in Section 2 and compare the results with other formulations in Section 3.

2. Formulation

We shall consider the following anharmonic oscillator Hamiltonian H

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^4 \tag{1}$$

to bring out the essential steps of the formulation. In eq. (1), p, x are linear momentum and position operators and $\lambda > 0$, a coupling parameter.

The first step in modifying the perturbation theory is to split H in the following two parts [3]

$$H_0 = \frac{1}{2}p^2 + \frac{1}{2}(1+2\beta)x^2, \tag{2a}$$

$$V = \lambda x^4 - \beta x^2, \tag{2b}$$

where β is a parameter. H_0 being harmonic oscillator Hamiltonian, its eigenvalues ε_n and eigen functions ϕ_n can explicitly be written down as a function of β. The interaction V mixes the states ϕ_n.

Following the work of Franchuk and Komarov [4], the parameter β is given by the cubic equation,

$$\beta^2(1+2\beta) - 9\lambda^2 = 0. \tag{3}$$

The modification given by (2a) and (2b) has also been used by Killingbeck [5]. It has also been shown to give good results for screened Coulomb potential problem [6]. In section 3 we shall give more details when we compare our calculation with the earlier ones.

Eq. (3) has a simple solution when $\lambda \to \infty$. It is given by

$$\beta = \frac{1}{2}(6\lambda)^{2/3}. \tag{4}$$

In the further development of the present formulation, we shall only discuss the case of $\lambda \to \infty$. Of course if one wishes, one can calculate the perturbed eigenvalues for other values of λ also by solving the cubic equation (3).

Before we proceed further, we would like to remark that rescaling in perturbation theory has earlier been studied by Banerjee [7] and finding a more convenient zero-order Hamiltonian by Bhattacharya [8], who has also looked into summing a divergent series using Euler transformation. The method which we propose here is different than these two methods and gives very accurate values even in the lower orders of perturbation.

Introducing the new variable ξ, given by

$$\xi = (6\lambda)^{1/6} x, \tag{5}$$

We can write the new unperturbed H_0 and perturbation potential V as

$$H_0 = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2, \tag{6a}$$

$$V = \frac{1}{6}\xi^4 - \frac{1}{2}\xi^2. \tag{6b}$$

The ground state eigenvalue E_0 of H when $\lambda \to \infty$ is given by

$$E_0 = (6\lambda)^{1/3}\omega_0, \tag{7}$$

ω_0 being the eigenvalue of $H_0 + V$ given by (6a) and (6b).

We denote the eigen functions of H_0 given by (6a)by $\chi_n(\xi)$. The next important step in writing the R–S perturbation theory in a new form is to introduce a set of variational parameters g_n in (6a) and (6b) as follows :

$$H_0 = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2 + \sum g_n |\chi_n\rangle\langle\chi_n|, \tag{8a}$$

$$V = \frac{1}{6}\xi^4 - \frac{1}{2}\xi^2 - \sum g_n |\chi_n\rangle\langle\chi_n|. \tag{8b}$$

It will now be shown how to use these variational parameters, so that the lowest orders of R–S perturbation theory provide fairly accurate values of the perturbed energies.

The contributions in various orders to ω_0 are denoted by $\omega_0^{(r)}$. The expression for $\omega_0^{(r)}$ can easily be written down from the ones given for R-S perturbation theory [1] by replacing the unperturbed energies by $\varepsilon_n + g_n$ where $\varepsilon_n = (n + \frac{1}{2})$ and subtracting g_n in the diagonal matrix elements $\langle n|V|n\rangle$ of perturbation potential. Thus, the zeroth, first, second and third order contributions are given by :

$$\omega_0^{(0)} = \frac{1}{2} + g_0, \tag{9a}$$

$$\omega_0^{(1)} = v_{00} - g_0, \tag{9b}$$

$$\omega_0^{(2)} = -\frac{v_{04}^2}{\left(\frac{9}{2} + g_4\right) - \left(\frac{1}{2} + v_{00}\right)}, \tag{9c}$$

$$\omega_0^{(3)} = -\frac{v_{04}^2 (v_{44} - g_4)}{\left[\left(\frac{9}{2} + g_4\right) - \left(\frac{1}{2} + v_{00}\right)\right]^2}. \tag{9d}$$

in the above $v = \frac{1}{6}\xi^4 - \frac{1}{2}\xi^2$,

$$v_{nm} = \langle\chi_n| v |\chi_m\rangle.$$

For these low order contributions, the parameters g_0 and g_4 can be obtained by making the odd terms $\omega_0^{(1)}$ and $\omega_0^{(3)}$ vanish. This gives $g_0 = \nu_{00}$ and $g_4 = \nu_{44}$. Using these values we can write

$$\omega_0^{(0)} = \frac{1}{2} + \nu_{00}, \tag{10a}$$

$$\omega_0^{(2)} = -\frac{\nu_{04}^2}{\left[\left(\frac{9}{2} + \nu_{44}\right) - \left(\frac{1}{2} + \nu_{00}\right)\right]}. \tag{10b}$$

Expressions (10a) and (10b) as one can easily see, are exactly the same as one gets in B-W theory where one replaces the perturbed energy by H_{00}.

Putting in the numerical values of ν_{04}, ν_{44} in expressions (10a), (10b) and using expression (7), we find that the ground state energy E_0 upto third order of perturbation is given by

$$E_0 = \frac{31}{84}(6\lambda)^{1/3}. \tag{11}$$

This is the same value which was obtained by Franchuk and Komarov [4] using creation and annihilation operators and separating the total Hamiltonian in terms of commuting and non-commuting parts.

We would next like to show that the present formulation also gives excellent results for the excited states. We consider the first excited state of the anharmonic oscillator given by expression (1). For the first excited state the condition

$$\langle \phi_1 | V | \phi_3 \rangle = 0, \tag{12}$$

leads to the following Franchuk-Komarov like equation for the parameter β,

$$\beta^2(1+2\beta) - 25\lambda^2 = 0 \tag{13}$$

which has the solution

$$\beta = \left(\frac{25}{2}\right)^{1/3} \lambda^{2/3} \tag{14}$$

when $\lambda \to \infty$.

The new variable ξ is now related to x as

$$\xi = (10\lambda)^{1/6} x. \tag{15}$$

The unperturbed Hamiltonian is again given by expression (6a), while the perturbation V is given by

$$V = \frac{1}{10}\xi^4 - \frac{1}{2}\xi^2. \tag{16}$$

The energy of the first excited state E_1 of H when $\lambda \to \infty$ is given by

$$E_1 = (10\lambda)^{1/3}\omega_1, \tag{17}$$

ω_1 being the value of the first excited energy state of H given by (6a) and (16).

One can now carry through the same perturbative calculation for ω_1 as was done earlier for ω_0. We have carried through this calculation, upto third order only. This gives us the energy E_1 of the first excited state to be

$$E_1 = \frac{69}{62}(10\lambda)^{1/3} = 2.39768\lambda^{1/3}. \tag{18}$$

Comparing this with the very accurate value of E_1 calculated by Hioe and Montroll [9] we find that the percentage error is 0.17%.

Thus, the formulation gives fairly accurate values of the excited states also. It will be worth exploring further, why the condition $\langle\phi_1|V|\phi_3\rangle = 0$ leads to such excellent results.

3. Concluding remarks

We have shown, how to reformulate R-S perturbation theory using additional parameters so that its few low-order terms give a fairly accurate value of the ground and excited state of the anharmonic oscillator when the coupling parameter $\lambda \to \infty$. Our procedure involves two steps. In the first step, the unperturbed Hamiltonian H_0 is written as a function of an unknown parameter which is determined by Franchuk-Komarov type equation. The same kind of splitting of total Hamiltonian has been done by Killingbeck [5], but he determines the unknown parameter by taking the derivative of the calculated energy upto a certain order and putting it equal to zero. In Franchuk and Komarov's formalism [4], it is determined by minimizing the zero-th order energy. Our calculated ground state energy upto second order is the same as the one obtained by Franchuk and Komarov [4]. The new form as developed here, has the advantages of the usual R-S perturbation theory as well as giving very accurate results for ground and excited states even when the strength of the interaction become very large.

References

[1] G Baym *Lectures on Quantum Mechanics* (New York Benjamin) Ch 11 (1969), C H Wilcox *Ed Asymptotic Perturbation Theory and its Applications in Quantum Mechanics* (New York . John Wiley) *Articles by* J O Hirschfelder p 3 and S T Epstein p 49 (1966)

[2] C A Arteca, F M Fernandez and E A Castro *J. Math. Phys* **25** 2377 (1984), *ibid* **25** 3492 (1984)

[3] N Ullah *Pramana-J. Phys* **24** 27 (1985)

[4] I D Franchuk and L I Komarov *Phys. Lett.* **88A** 211 (1982)

[5] J Killingbeck *J. Phys.* **A14** 1005 (1981)

[6] N Ullah *Phys. Rev* **A33** 723 (1986)

[7] K Banerjee *Proc. Roy. Soc* (London) **A368** 155 (1979)

[8] K Bhattacharya *Int. J. Quant. Chem.* **20** 1273 (1981), *ibid* **22** 307 (1982)

[9] F T Hioe and E W Montroll *J. Math. Phys.* **16** 1945 (1975)